REPORT DOCUMENTATION PAGE	*Form Approved* *OMB No. 0704-0188*

1. REPORT DATE *(DD-MM-YYYY)*	2. REPORT TYPE	3. DATES COVERED *(From - To)*
27-01-2012	Final	Apr 2004 - Sept 2011

4. TITLE AND SUBTITLE

Center of Excellence in Hypersonics Research

5a. CONTRACT NUMBER

5b. GRANT NUMBER

FA9550-10-1-0352

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)

Candler, Graham, V
Mahesh, Krishnan
Schwartzentruber, Thomas

Holden, Michael
MacLean, Matthew

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

University of Minnesota, 110 Union Street SE, Minneapolis, MN 55455

CUBRC Inc., 4455 Genesee Street, Buffalo, NY 14225

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

Air Force Office of Scientific Research
875 North Randolph Street Suite 325
Arlington, VA 22203

10. SPONSOR/MONITOR'S ACRONYM(S)

AFOSR

11. SPONSOR/MONITOR'S REPORT NUMBER(S)

AFRL-OSR-VA-TR-2012-0792

12. DISTRIBUTION/AVAILABILITY STATEMENT

Unlimited

13. SUPPLEMENTARY NOTES

14. ABSTRACT

The Center of Excellence in Hypersonics Research was established to support future hypersonic vehicle development programs. The Center engaged leading experts in experimental and computational analysis of hypersonic flows to provide research, education, and technology development in hypersonics. The Center combined the world’s premiere hypervelocity testing facility at the CUBRC with state-of-the-art computational simulation methods at the University of Minnesota to rapidly advance the field of hypersonics. The Center supported fundamental research in hypersonics, including the development of high-quality experimental databases for code testing and validation of prediction tools. Many of these codes have been transferred to government and industry to enable optimized hypersonic vehicle designs. The Center also supported a rigorous graduate program that transferred technical capabilities from the previous generation of hypersonics experts to new students in the field. This helped preserve the nation’s dwindling talent pool and provided a source of scientists and engineers for future research and development programs.

15. SUBJECT TERMS

hypersonic flow, computational fluid dynamics, hypersonic aerodynamics, air-breathing propulsion

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Candler, Graham, V
U	U	U	UU	45	19b. TELEPHONE NUMBER *(Include area code)* 612-625-2364

Reset

FINAL REPORT

CENTER OF EXCELLENCE FOR HYPERSONICS RESEARCH

AFOSR FA9550-04-1-0341
AFOSR FA9550-10-1-0352

Graham Candler
Krishnan Mahesh
Thomas Schwartzentruber
Department of Aerospace Engineering and Mechanics
University of Minnesota
Minneapolis, MN 55455

Phone: 612-625-2364; Fax: 612-626-1558
Email: candler@aem.umn.edu, mahesh@aem.umn.edu, schwartz@aem.umn.edu

Michael Holden
Matthew MacLean
Calspan – University at Buffalo Research Center
Buffalo, NY

Phone: 716-631-6853; Fax: 716-631-4117
Email: holden@cubrc.org, maclean@cubrc.org

January 25, 2012

ABSTRACT

The Center of Excellence in Hypersonics Research was established to support future Department of Defense and NASA hypersonic vehicle development programs. The Center engaged leading experts in experimental and computational analysis of hypersonic flows to provide research, education, and technology development in hypersonics. The Center combined the world's premiere hypervelocity testing facility at the Calspan – University at Buffalo Research Center with state-of-the-art computational simulation methods at the University of Minnesota to rapidly advance the field of hypersonics. The Center supported fundamental research in hypersonics, including the development of high-quality experimental databases for code testing and validation of prediction tools. Many of these codes have been transferred to government and industry to enable optimized hypersonic vehicle designs. The Center also supported a rigorous graduate program that transferred technical capabilities from the previous generation of hypersonics experts to new students in the field. This helped preserve the nation's dwindling talent pool and provided a source of scientists and engineers for future research and development programs. The Center of Excellence in Hypersonics Research was a national focal point for U.S. research and training in hypersonics.

INTRODUCTION

The major programs currently being undertaken by the Department of Defense and NASA to develop new advanced hypersonic vehicles and space access systems will require significant advances in the design methods and ground testing techniques to ensure successful flight testing. In the period from 1950 to 1970, the U.S. led the world in the development of space access systems and hypersonic vehicle design. However, the past decade has seen the loss and retirement of many of the talented personnel trained in this era and a dearth in research to resolve key problems associated with aerothermal problems arising in hypersonic vehicle design. Exacerbating this problem has been the lack of funding to train new scientists in this area and the development of numerical and experimental techniques to provide accurate models of the aerothermodynamic processes used in the methods to design and analyze hypersonic vehicles employing revolutionary designs. Such is the status of this area that there is significant question as to whether currently America has the engineering talent to rapidly replicate the activities in the 1960s which placed American astronauts on the moon. These observations motivated the need for a Center of Excellence in the area of hypersonic flows to advance the state of the art in the understanding of hypersonic flows over vehicles and to train the scientists and engineers who will design these future hypersonic vehicles.

Under AFOSR funding, we established a partnership between the University of Minnesota and the Calspan – University at Buffalo Research Center (CUBRC) to develop a Center of Excellence in Hypersonic Research. CUBRC has the world's premiere hypersonic/hypervelocity testing facilities and unique hypervelocity instrumentation developed over 40 years of wind tunnel testing at hypersonic flight conditions. The University of Minnesota has state-of-the-art capabilities to simulate hypersonic flows including laminar complex regions of shock/boundary layer interaction and flow chemistry, transition to turbulence, finite-rate air and combustion chemistry, turbulent mixing in compressible flows, and shock wave/turbulent boundary layer interactions. The research supported by AFOSR through the Center has greatly advanced the ability to accurately test and simulate hypersonic flows.

The Center trained many young engineers and scientists to conduct experimental research in state-of-the-art hypersonic test facilities at CUBRC, and perform numerical simulation and analysis with the most advanced numerical codes and modeling techniques at the University of Minnesota. A major research focus was a program of combined numerical and experimental analysis to investigate key phenomena associated with the performance of re-entry vehicles, airbreathing propulsion systems, and hypersonic interceptors. Employing its unique combination of large-scale test facilities and efficient computational simulation methods the Center stimulated advances in the aerothermodynamics of hypervelocity flows, leading to improved methods to design, analyze and evaluate the performance of new hypersonic vehicles and airbreathing propulsion systems.

OBJECTIVES AND APPROACH

The objective of the Center of Excellence in Hypersonics was to develop a strong research and training program in hypersonics to support the Nation's future hypersonic vehicle development. The Center drew on the extensive experience of the principal investigators in hypersonic ground testing, numerical simulation, graduate student advising, and classroom teaching. The Center was a national focal point for academic research and training in the U.S.

The Center of Excellence in Hypersonics Research combined fundamental research, education, and technology development to support the nation's future hypersonic vehicle development. The primary mission of the Center was to perform research on critical problems in the field, such as real gas effects, shock wave – turbulent boundary layer interactions, transition to turbulence, and scramjet testing and simulation. The research program was used to drive the academic mission of the Center, which was to train a new generation of hypersonics experts. This was accomplished through relevant course work, hands-on computational method development, design and testing of experiments, and computational analysis of experimental results.

KEY ACCOMPLISHMENTS

The AFOSR Center of Excellence in Hypersonics Research was a large-scale multi-year effort that resulted in a very large number of publications; these are listed below. It is not possible to provide detailed information about each sub-topic of the research accomplished under this program. Rather, in this section we provide key highlights of the research and refer the reader to the publications for additional details. We organize the work into several major topics:

1. Development of advanced numerical methods and codes for high-speed and hypersonic flow simulations.
2. Development of two-dimensional, axisymmetric and fully three-dimensional boundary layer stability analysis tools.
3. Detailed experimental measurements to provide validation data for hypersonic flow simulations.
4. Hybrid RANS-LES simulations and direct numerical simulations of transitional and turbulent hypersonic flows.

5. Advanced particle-based simulation methods (Direct Simulation Monte Carlo and molecular dynamics) for hypersonic rarefied flows

Each of these topics has produced many papers and several Ph.D. theses over the course of the Center program. In many ways, this work leads the field and it would not have been possible without the AFOSR support of the Center. Much of this work has been transitioned to Air Force Research Laboratories and to other national labs and industry.

Advanced Numerical Methods for Hypersonic Flow Simulations

The standard numerical simulation approach for high-speed shock-dominated flows has been based on upwind-biased Riemann solvers since the early days of computational aerodynamics. These numerical flux functions are very effective at providing stable, robust simulations of steady-state hypersonic flows including the effects of chemical reactions. However, these methods stabilize the flow by adding large levels of numerical dissipation – simply put, the upwind flux functions smear out discontinuities and cause small-scale unsteady motion (kinetic energy) to be converted to thermal energy. Thus, when these methods are used to simulate unsteady flows, they artificially dissipate the small-scale (both in length and time) unsteadiness. To accurately resolve an unsteady flow with these methods would require impractically large grids, especially as the Reynolds number approaches realistic flight conditions. Therefore, two new classes of methods were developed under Center support.

Two approaches were taken. In the Candler group, a new numerical flux function was developed that conserves a secondary quantity, in this case kinetic energy [63]. For a compressible flow, kinetic energy is not actually conserved, so for compressible flows this approach is consistent with kinetic energy conservation. Namely, the resulting discrete flux of kinetic energy is consistent with the kinetic energy conservation equation. This approach was shown to significantly reduce the numerical dissipation for standard numerical test cases. For example, the method produces the expected behavior as a function of Reynolds number for the decay of weakly compressible and highly compressible isotropic turbulence. With the careful addition of dissipation to control behavior near strong shock waves and density gradients, the kinetic energy consistent method has been applied to a wide array of practical problems. These will be discussed in more detail below.

Recently, the kinetic energy consistent fluxes have been extended to fourth and sixth order accuracy for certain classes of grids. The theoretical order of accuracy can be achieved on weakly stretched hexahedral grids, as shown by numerical test cases. For practical problems that involve non-ideal grids, the higher-order formulations have been shown to produce clearly superior solutions than the lower order method. Thus, even though ideal performance is not always obtained, the higher-order methods are very useful for realistic problems; in many ways, they enable new classes of simulations of turbulent high-speed flows.

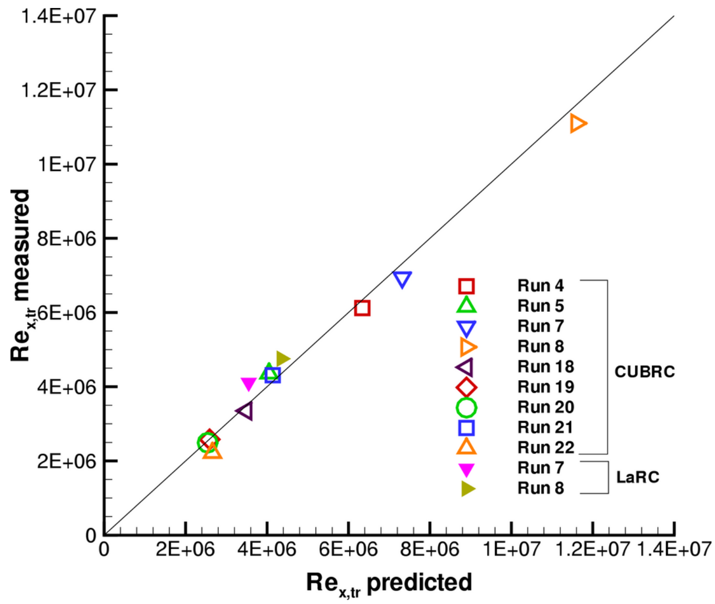
Work was also conducted to improve the time integration aspect of numerical simulations. A novel second-order modified Crank-Nicholson approach was developed and tested. For certain problems (e.g. jets in supersonic crossflow), the method extends the accuracy of the simulations allowing larger time steps to be taken for a given level of accuracy.

In the Mahesh group, a new approach that rescales the governing equations so that they become inherently less stiff (difficult to solve numerically) at low Mach numbers, yet still producing accurate results at high Mach number [17]. This approach is documented in the cited Journal of Computational Physics articles and has been applied to numerous compressible flow problems.

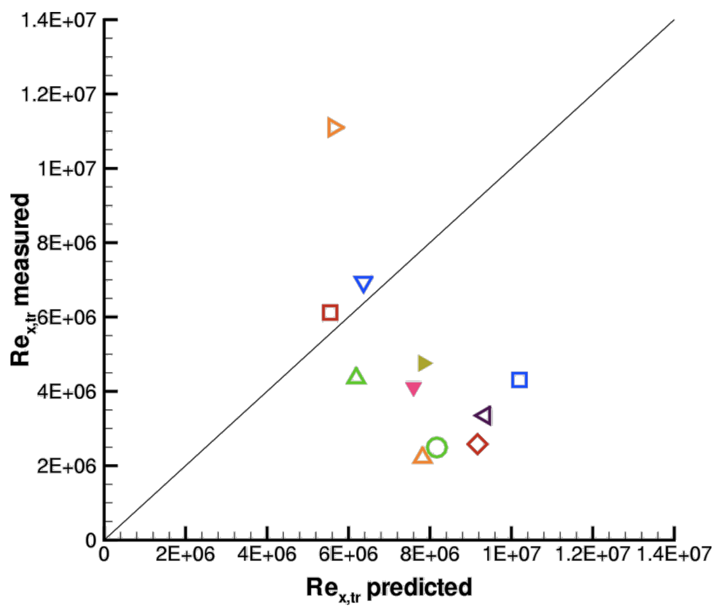
Both approaches have been implemented in large-scale, highly-parallel computational fluid dynamics codes. The US3D code [5, 11] has been transitioned to several AFRL sites including Wright-Patterson AFB (Air Vehicles Directorate) and Kirtland AFB (Space Vehicles Directorate). This code includes many key features for practical flow simulations: general thermo-chemical model for high-enthalpy nonequilibrium flows, laminar and RANS transport models, capability of rapid convergence to steady-state using implicit methods and upwind fluxes or time-accurate mode with low-dissipation kinetic energy fluxes and higher-order time accurate integration methods, the ability to handle hybrid unstructured grids composed of a mix of tetrahedral, pyramids, prisms, and hexahedral grid elements. (Though hexahedral grids are generally preferred for accuracy reasons.) A critical aspect of the work involved designing the code to be scalable to large numbers of processing elements (CPUs or CPU cores) so that very large simulations can be performed. This required careful attention be paid to input/output processes which can be a serious limitation for large grids; the code reads and writes in parallel and does dynamic partitioning to make it efficient and flexible. It has been run successfully on 4000 processing elements on a 500 million element grid. There is no inherent reason that it should not scale beyond this problem size.

Development of Tools for Hypersonic Boundary Layer Stability Analysis and Prediction

A key accomplishment from the Center was the development of the STABL suite of codes for hypersonic boundary layer stability analysis (STABL = Stability and Transition Analysis for hypersonic Boundary Layers) [12, 24, 60]. The primary component of the STABL code is a parabolized stability equations (PSE) solver for high-enthalpy flows; this code can be run in parallel to reduce simulation times and it can be driven with an intuitive graphical user interface so that non-experts can run analyses and interpret the data. It includes a full thermo-chemical model for nonequilibrium flows so that the effects of finite-rate chemical reactions and internal energy relaxation can be included in the stability analysis. In addition, STABL includes a parallelized computational fluid dynamics code that is set up for rapid mean flow solutions to support the stability analyses. However, STABL is limited to two-dimensional and axisymmetric problems; though it has been run successfully on symmetry planes of more complex three-dimensional hypersonic flows. STABL is in wide use by US national labs, academia, and industry; it is the de facto standard for stability analyses of hypersonic flows. It was used to support the design of the AFRL HIFiRE Flight Experiments (flights 1 and 5) [34, 46-48, 50, 69], to analyze the X-43 post-flight data, to provide predictions of transition to turbulence on the DARPA HTV-2 re-entry vehicle [56], and it is has been and is currently being used to correlate Sandia National Laboratories flight data, among other programs. An example of the utility of the STABL code is shown in Fig. 1, which plots the predicted transition location versus the measured transition location for two prediction methods – the conventional correlation of Reynolds number based on momentum thickness over boundary layer edge Mach number and the present mechanism-based approach the uses stability theory to compute the growth of disturbances and correlates their integrated growth to wind tunnel data (the e^N method). This result is for the HIFiRE-1 blunt cone configuration in the CUBRC and NASA Langley wind tunnels. Note that the traditional approach has very limited predictive capability, while the mechanism-based approach correlates the diverse data very well.



(a)



(b)

Figure 1. Predicted vs. measured transition location on the HIFiRE-1 blunt cone using two approaches: (a) the mechanism-based STABL calculation and the N-factor approach with N = 5.5; (b) the $Re\theta$ / M_e = 150 empirical approach.

A three-dimensional version of STABL was developed under Center support. This code required a complete reformulation and rewrite of the stability solver. It is now being extended to include a graphical user interface and features that will make is useful to the user community.

Experimental Data for Code Validation

An important and extensive component of the Center was collaborative computational and experimental research to develop high-quality validation data for high-enthalpy flow simulation codes [1, 3, 5, 7, 8, 10, 32, 39, 83, 84]. This work largely focused on the double-cone and hollow-cylinder-flare configurations that have been the subject of code validation studies. In addition, the test-section conditions in the CUBRC LENS-I reflected shock tunnel facility were characterized at a new level of detail. Laser diagnostics systems were used to measure nitric oxide (NO) levels to be measured in the LENS facilities test-sections [9, 22, 40]. This work was tightly coupled with numerical simulations to maximize the benefit of the diagnostics work. Critical new results were obtained for mixtures of argon and oxygen at a range of enthalpies for the double-cone flow (discussed in more detail below). These measurements show that the lack of agreement between simulation and experiment at high enthalpy is due to the dissociation of oxygen in the facility reservoir; present thermo-chemical models for the expansion of this reacted gas through the facility nozzle are inadequate and must be missing some key physical process or processes. In particular, it is possible that the low-lying electronically excited states of oxygen may play a role in the recombination process; work is continuing in the attempt to better model the recombination process [80, 85]. In the following, we highlight some results from the recent double-cone experiments and related simulations.

High Enthalpy Measurements on 25^o/55^o Double Cone

In response to observed limitations in correctly computing the laminar separated flowfield over a 25^o/55^o double cone geometry (shown in Fig. 2), a number of new experiments were performed targeting two areas of particular difficulty regarding the ability of simulations to reproduce experimental measurements. The first set of experiments targeted a computational unsteadiness observed at selected high enthalpy nitrogen conditions. The second area responded to limitations in the modeling of high enthalpy air chemistry by generating additional data using mixtures of oxygen and argon as a test gas, thereby eliminating the Zeldovich exchange processes (involving nitric oxide) from the physics of the flow field. The test conditions for these two series of tests are listed in Table 1.

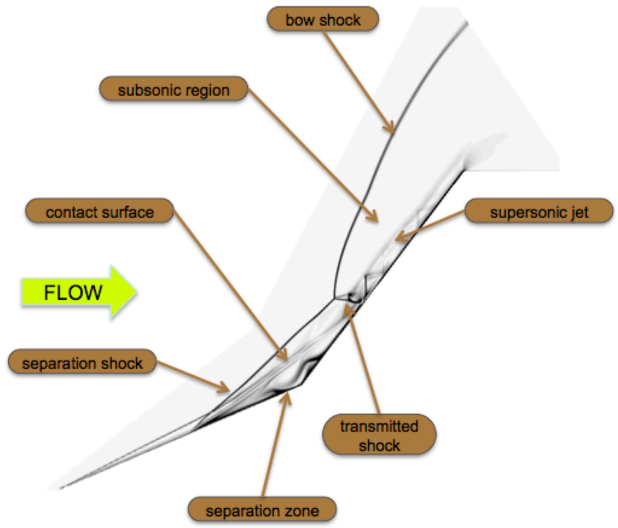
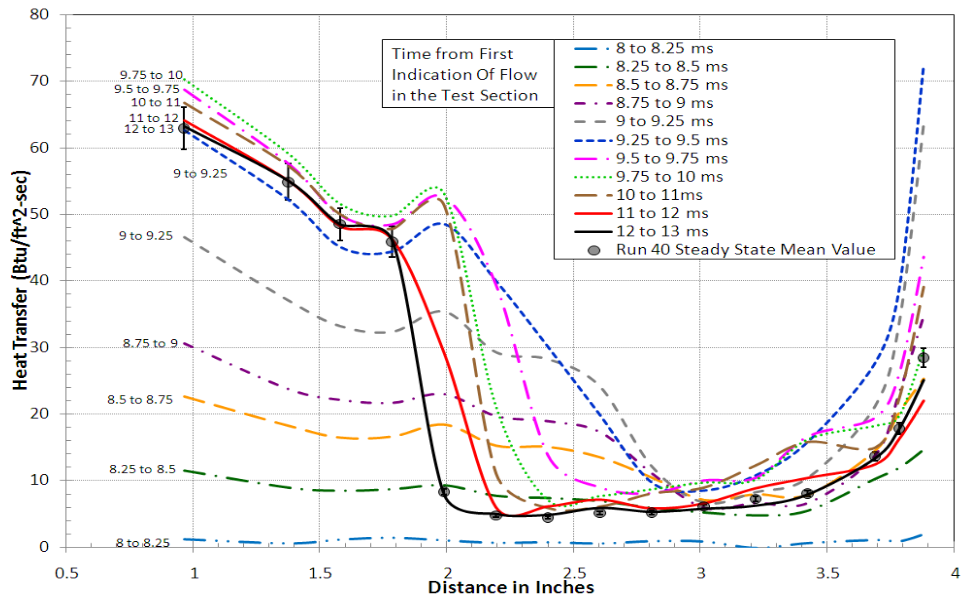
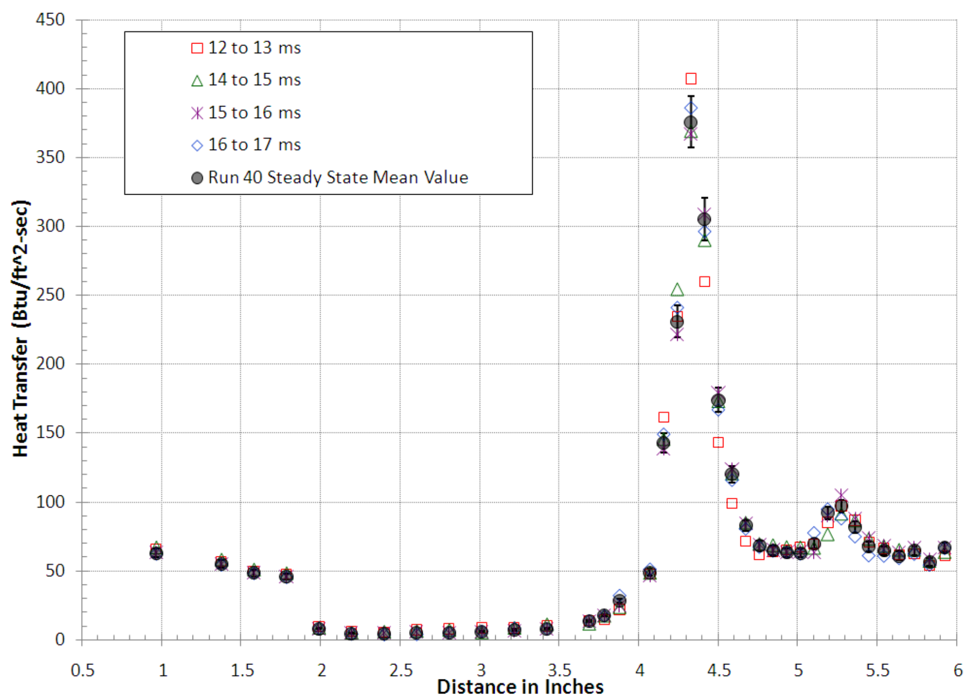


Figure 2. Flowfield over $25^{O}/55^{O}$ double cone

During the course of a recent RTO validation study, Run 40, a double cone test case run at high Reynolds numbers under high temperature conditions with a nitrogen flow, was selected for code validation studies. In retrospect, this choice proved unfortunate because while the similar measurements in air were computed successfully, and a stable flow was predicted, in our program no such computations were attempted for the equivalent run conducted in nitrogen – Run 40. The heat transfer and pressure measurements made over the double cone configuration in Run 40 demonstrated that a steady separated region was formed within 4 ms of the flow initiation over the model (Figure 3(a)) and remained steady for another 4 ms as illustrated in Figure 3(b). Figure 3(b) illustrates that a large separated region is formed at the cone/flare junction with a well-defined heating peak in the reattachment region followed by a large region well-defined attached flow at the trailing edge of the flare. There are no indication from the surface heat transfer and pressure measurements or from the high-speed video that the separated region is increasing in size beyond its proportions at 12 ms. However, for this test condition, a number of computationalists have obtained solutions where the separated region increases in size with time despite the fact that experiment showed no such flow instability.



(a)



(b)

Figure 3. Temporal variation of the heating distribution during separated flow establishment at the double cone junction for Run 40

The detailed investigation by Nompelis, et al. [84] revealed that, for his computational method, the boundaries between stable and unstable solutions could be plotted in terms of the characteristic Reynolds number and the freestream total enthalpy, as shown in Figure 4, which indicate that decreasing the Reynolds number or increasing freestream enthalpy results in a predicted stability of the separated region across a well-defined bounding curve.

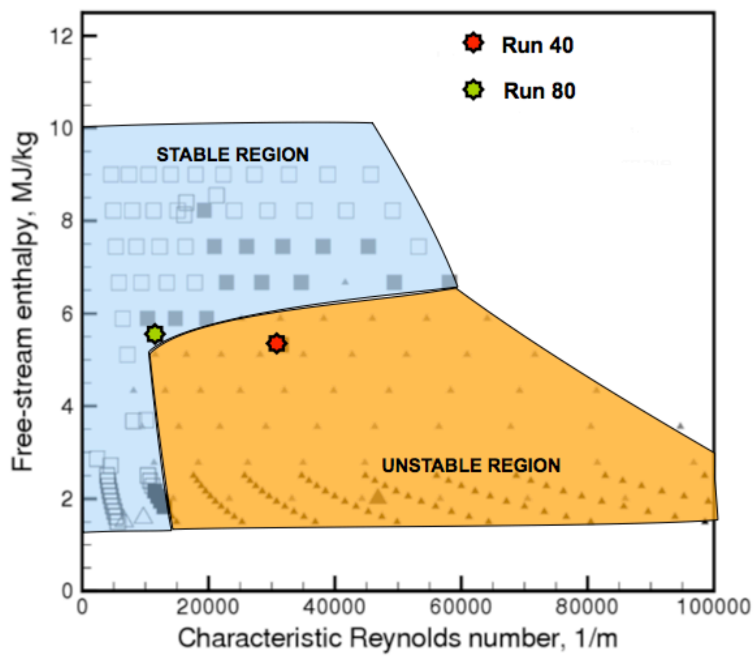
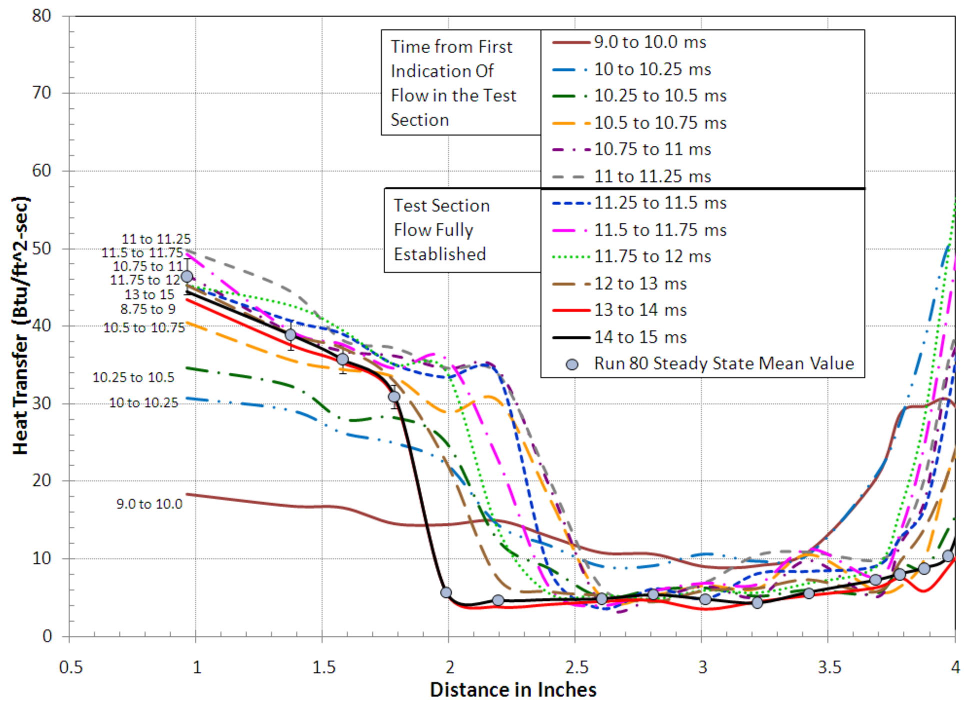
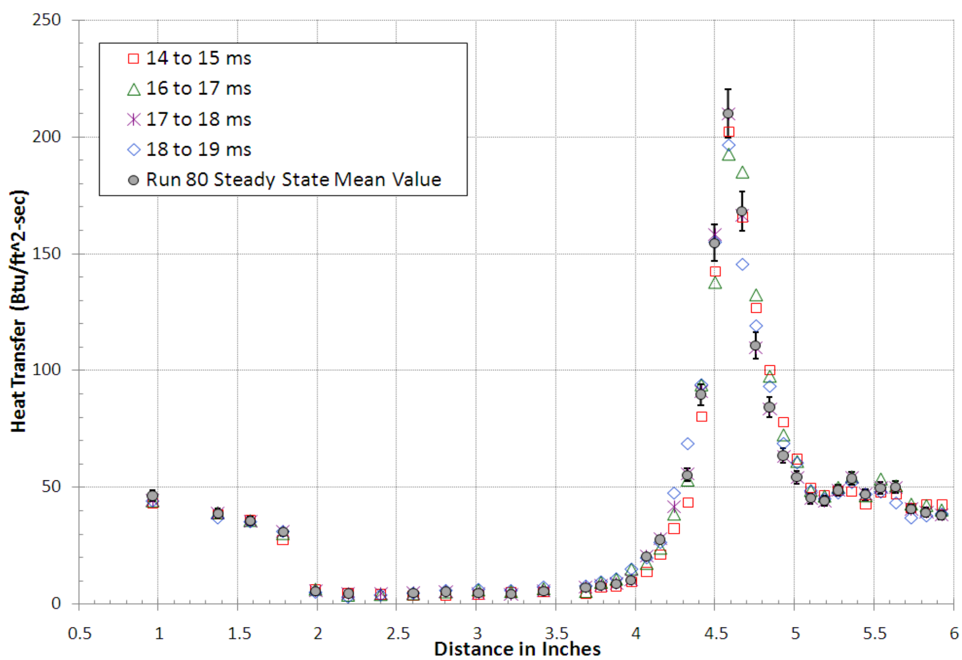


Figure 4. Nompelis's calculations defining the boundaries for stable and unstable N-S solutions

Based on these calculations we selected additional high-enthalpy test cases with a nitrogen freestream flow. From these runs we selected (Run 80) which was run at a total enthalpy of 5 MJ/kg and a unit Reynolds number half that of Run 40 to be the new code validation test case. Measurements of the development of the separated region for this test case is illustrated with the heat transfer measurements made in the interaction region over the fore- cone in Figure 5(a). For this condition the flow is established in the test section in approximately 1.25 ms and the separated region over the model reaches a stable size in approximately 4 ms after that. As illustrated in Figure 5(b), the separated region remains stable in size for the following 5 ms during the remaining steady test flow through the tunnel.



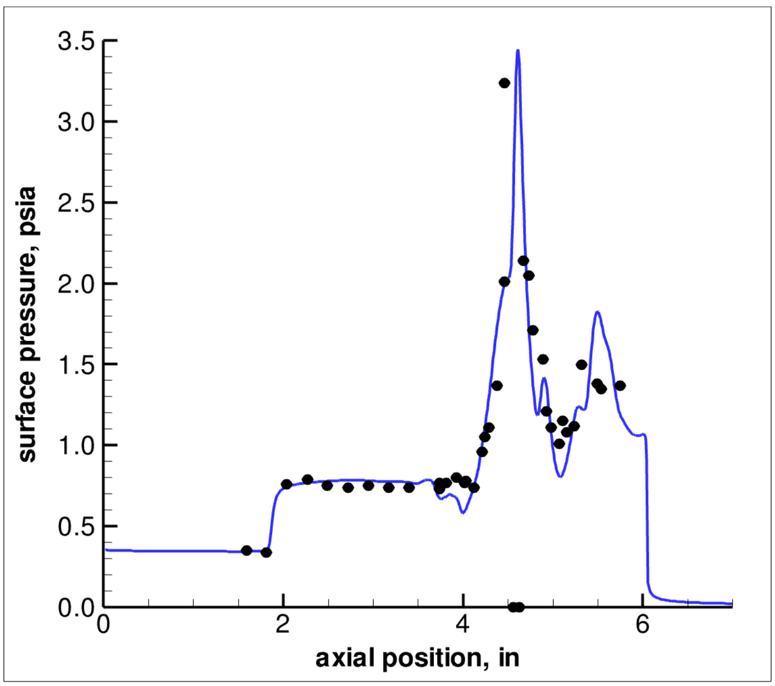
(a)



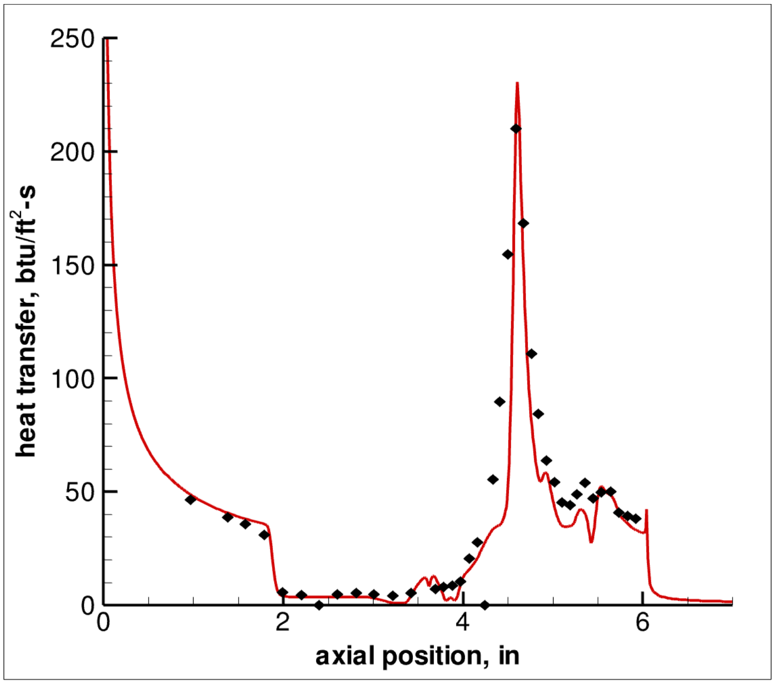
(b)

Figure 5. Temporal variation of the heating distribution during separated flow establishment at the double cone junction for Run 80

The predictions made by Nompelis, (which are similar to those obtained by MacLean at CUBRC with the DPLR code), reach steady levels in approximately the same flow times as measured by experiment and do not indicate that the separated region grows further with increasing time. Comparisons between the measurements and Nompelis pre-test predictions of heat transfer and pressure through the interaction regions are shown in Figure 6. Here we see excellent agreement between prediction and measurements. Clearly this test case (Run 80) should provide a more viable code validation data set than Run 40 for CFD validation and development.



(a)



(b)

Figure 6. Steady state distribution of pressure and heat transfer over the double cone

A serious limitation in the capability to predict high enthalpy flow over the double cone using reacting air as a test medium was shown by Center researchers. In response the these findings, a series of new experiments have been performed to eliminate the uncertainty associated with modeling the formation of nitric oxide where oxygen and oxygen/argon mixtures were used as a test gas. These tests used pure oxygen at several enthalpy levels and mixtures of various percentages of oxygen diluted with argon to isolate the kinetics of oxygen dissociation alone.

The comparison between theory and experiment for the first set of measurements made in pure oxygen freestream with a total enthalpy of 4 MJ/kg are shown in Figure 7. As with air, excellent agreement is achieved between the heat transfer and pressure measurements and the predictions for flows where the nonequilibrium effects are small. However, when we increase the total enthalpy level in the freestream for a pure oxygen flow in Figure 8, again the length of the separated region is significantly underpredicted.

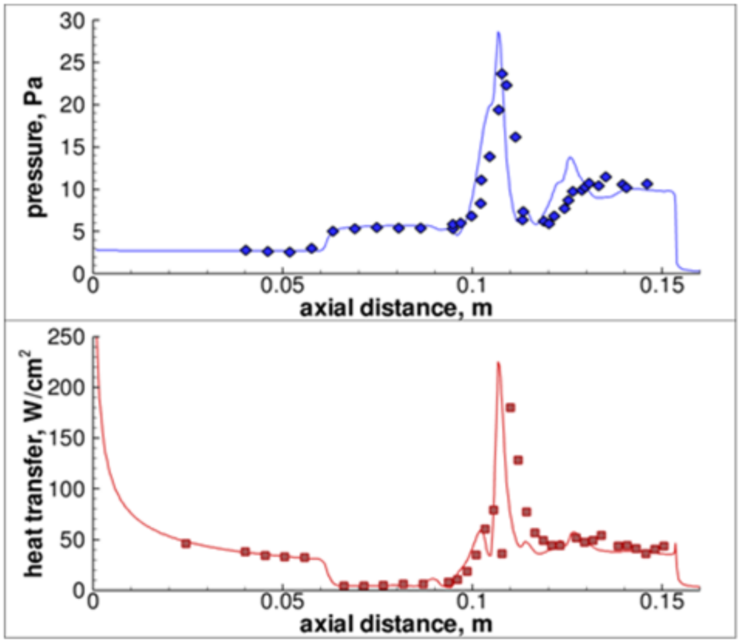


Figure 7. Comparison of heat transfer and pressure measurements with Nompelis Navier-Stokes predictions for 100% oxygen freestream at a total enthalpy of 4 MJ/kg

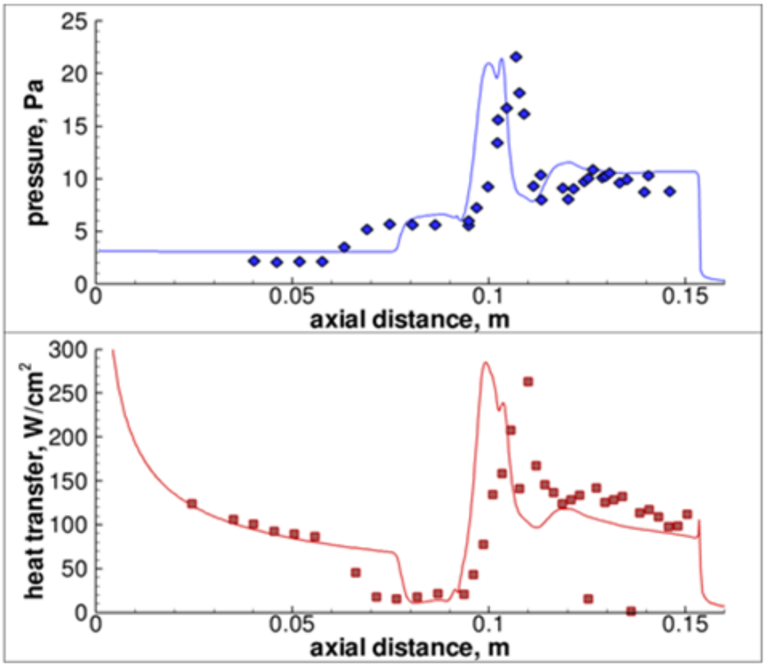
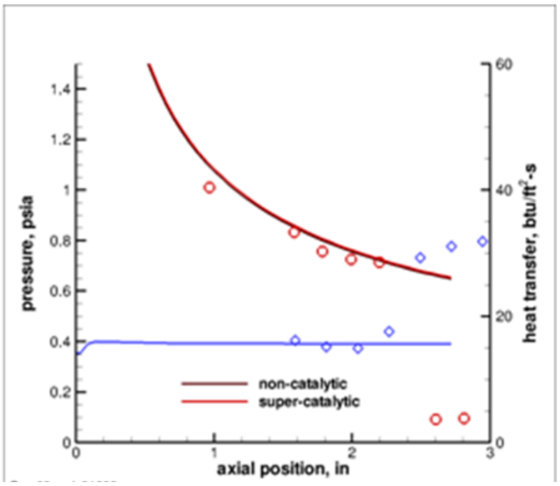


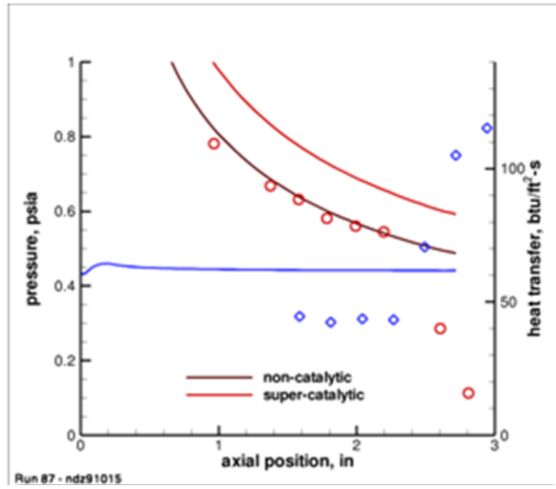
Figure 8. Comparison of heat transfer and pressure measurements with Nompelis Navier-Stokes predictions for 100% oxygen freestream at a total enthalpy of 10 MJ/kg

Of significant interest in the 10 MJ/kg test case is that the initial cone pressure significantly over-predicted where the flow is attached (as illustrated Figure 9(b)) which suggests that the calculation of the nozzle flow could be inadequate. This is a significant finding because the same models describing oxygen chemistry and thermodynamics that are used on the double cone are also used to predict the state of the freestream after expanding through the nozzle.

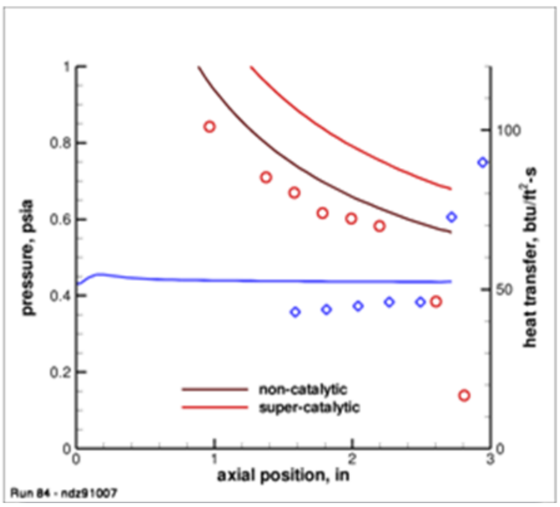
Decreasing the oxygen content improves the agreement in cone pressure as shown in Figure 9(c); however, the heating rate on the cone is over-predicted for both catalytic and non-catalytic boundary conditions. Increasing the density of the freestream flow, which implies an increase in the number of molecular collisions occurring in the expanding nozzle flow, significantly improves the agreement as shown in Figure 9(d). Clearly more accurate models are required to describe the chemistry in the freestream before we can evaluate the accuracy of the models of flow chemistry needed to describe the shock layer flows over the double cone. Further detailed flowfield measurements are required to resolve this problem and our major emphasis in the future will be investigating these flows in the expansion tunnel where the conditions will be selected to obtain flows with negligible nonequilibrium in the freestream.



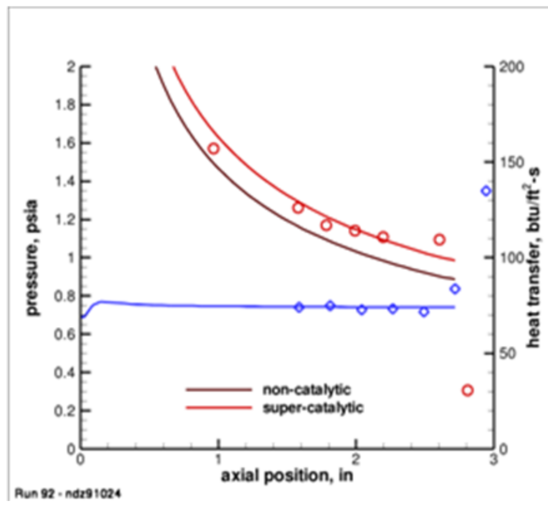
(a) 100% O2 / 4 MJ/kg



(b) 100% O2 / 10 MJ/kg



(c) 50% O2 – 50% Ar / 10 MJ/kg



(d) 50% O2 – 50% Ar / 10 MJ/kg

Figure 9. Variation of pressure and heat transfer on forecone with total enthalpy and freestream static pressure

Table 1. Freestream conditions for double cone study

Run#	total enthalpy (MJ/kg)	pressure (Pa)	density (kg/m3)	temperature (K)	vibrational temperature (K)	velocity (m/s)	frozen Mach	cN2	cN	cO2	cO	cAr
78	3.48	38.5	0.0009894	131	2,425	2,456	10.5	1.000000	0.000000			
79	5.29	63.4	1.316E-03	162	2,690	3,073	11.8	0.999885	0.000115			
80	5.28	63.6	1.291E-03	166	2,711	3,067	11.7	0.999875	0.000125			
81	6.39	61.3	9.234E-04	276	760	3,400	10.8			0.474165	0.025835	0.500000
82	8.1	100.5	1.045E-03	391	660	3,769	9.9			0.454586	0.045414	0.500000
83	5.12	35.9	7.396E-04	163	2,849	3,003	11.5	0.999824	0.000176			
84	9.27	109.3	9.621E-04	452	647	3,973	9.6			0.433079	0.066921	0.500000
85	10.17	145.7	9.243E-04	586	687	4,088	8.5			0.665478	0.084522	0.250000
87	9.85	164.8	9.422E-04	626	712	4,019	8.1			0.924517	0.075483	
88	8.78	165.3	1.061E-03	570	698	3,853	8.2			0.948209	0.051791	
90	3.99	90.7	1.834E-03	190	1,001	2,731	10.4			0.998556	0.001444	
91	10.26	311.5	1.550E-03	729	773	4,148	7.8			0.938891	0.061109	
92	8.77	205.0	1.722E-03	489	663	3,960	9.4			0.463152	0.036848	0.500000

High-Fidelity Simulations of Turbulent Flows: DNS, WM-LES and DES

A significant new capability for the simulation of turbulent flows was developed under the AFOSR Center of Excellence support. Conventional turbulent flow simulation approaches use Reynolds-averaged Navier-Stokes (RANS) methods, in which the unclosed turbulent transport terms are modeled using a turbulent viscosity and other effective turbulent transport coefficients. The models are designed to work for simple canonical flows and are then applied to complex practical problems. The RANS approach is known to work well for certain classes of problems such as attached subsonic boundary layer flows. However, it is seriously deficient for separated flows and recent experimental data obtained under Center support at CUBRC shows that two widely-used RANS models do not produce the correct heat flux for turbulent hypersonic flows.

As discussed above, a new numerical method was developed that significantly reduces numerical dissipation for compressible flows. This method enables a new class of simulations of turbulent high-speed flows. Namely, because the method does not artificially damp out small-scale motion, it can be used for simulations that resolve many (if not all) of the time-scales and length-scales of turbulent flows. This approach has been applied to base flows of re-entry vehicles, and to fuel-air mixing represented by a jet or jets in a supersonic cross-flow. This approach was also used to perform simulations of three non-trivial flows undergoing transition to turbulence [81, 88, 102, 104]. Ongoing work extends the approach to the direct numerical simulations of turbulent boundary layers, in which all scales are resolved by the simulation.

In the jet in cross-flow simulations, the approach used is a so-called wall-modeled large-eddy simulation or WM-LES. Here a RANS model (in this case the compressibility-corrected version of the Spalart-Allmaras model) is used near solid surfaces to provide a boundary condition to a large-eddy simulation (LES) that represents the large-scale turbulent motion away from the surface. This approach has been shown to be very effective for certain types of flows, and we have proven that it can reproduce the available experimental data for jets in supersonic cross-flow [21, 25, 28, 38, 55, 57, 71, 74, 89, 96, 99, 101, 108]. This is very important result because it paves the way for high-fidelity simulations of full combustors; work is now underway to use this approach for a representative geometry with multiple injectors at flight-relevant conditions. Figure 10 shows an image from a recent WM-LES of a rectangular duct with 5 angled injectors operating.

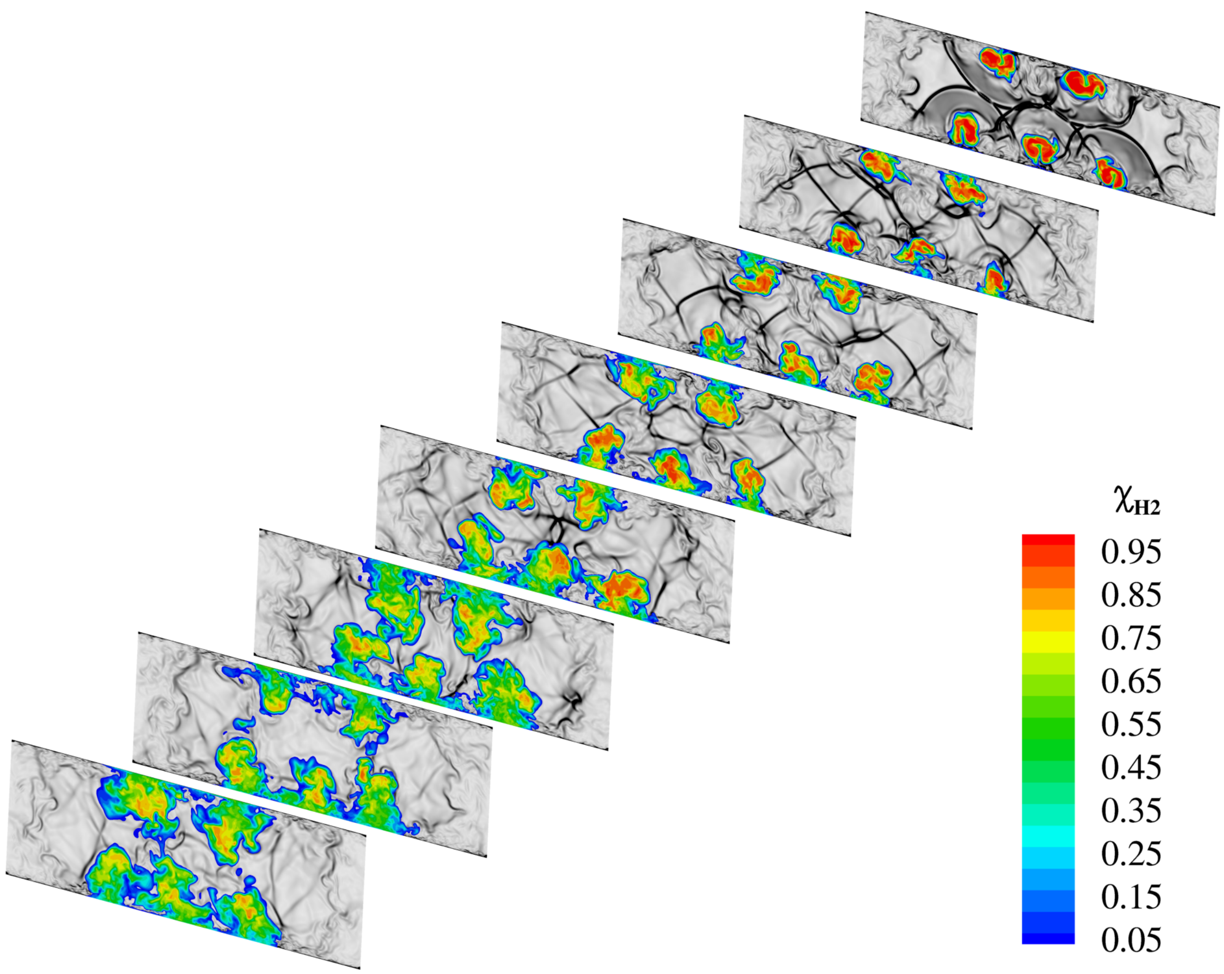


Figure 10. Hydrogen injection into a supersonic flow in a rectangular duct with 5 angled (30^o) injectors (mole fraction of H_2 in color, greyscale represents density gradient magnitude).

An additional capability that the low-dissipation numerical method enables is related to transition to turbulence in hypersonic flows. As discussed above, the STABL code and other stability analysis tools can correlate data for certain classes of problems. But there are many problems in transition physics that are not suitable to conventional stability analyses. Under Center support, we have applied the low-dissipation approach to the direct simulation of transition to turbulence for two problems: acoustic wave interactions with the Mach 8 flow over an elliptic cone at zero angle of attack and the instability growth in the wake of a discrete roughness element in a Mach 6 laminar boundary layer. These problems would not have been feasible without the low-dissipation numerical method and the work done under Center support to allow the code to scale to large numbers of processors and grid elements. Typical simulations use 1000 to 2000 cores and require 270 million element grids [88, 102].

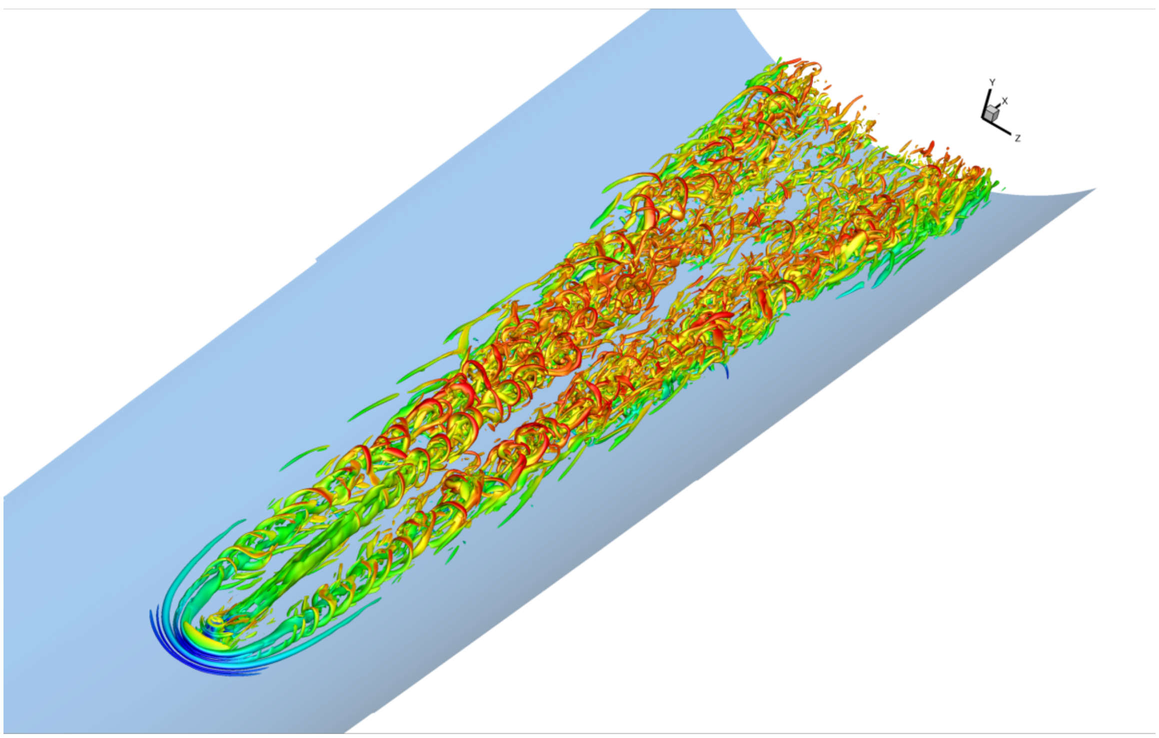


Figure 11. Isosurfaces of Q colored by velocity gradient magnitude in the wake of a cylindrical roughness element in a Mach 6 flow.

Figure 11 shows a result from the discrete roughness element simulation. Here, the roughness element is located at the lower left of the image, and is a cylindrical geometry protruding from the curved surface of a wind tunnel (the Purdue Mach 6 Quiet Tunnel). The variable plotted is Q, which is the second invariant of the velocity gradient tensor, and represents the location of vortical motion. The isosurfaces of Q are colored by the local velocity magnitude. Note that several vortices wrap around the roughness element and are then swept downstream. These interact with one another and ultimately cause the wake to break down to turbulent flow. Analysis and comparison with experimental measurements made at Purdue show that the wake has a dominant unsteadiness frequency (about 21 kHz in this case). We found that this dominant frequency is driven by the unsteady motion in the separation region ahead of the protuberance.

Advanced Particle-Based Simulation Methods for Hypersonic Rarefied Flows

AFOSR Hypersonics Center funding was used in Prof. Schwartzentruber's group for continued code development of a state-of-the-art particle simulation method for non-equilibrium gas flows. The method is called direct simulation Monte Carlo (DSMC) and some sample results are shown below. DSMC simulates the Boltzmann equation and is therefore accurate for flows ranging from continuum to free-molecular. The method is used to predict drag and heating environments for high-speed, high-altitude objects (satellites, space vehicles, etc.); regimes where the continuum fluid equations become inaccurate. DSMC moves millions of representative molecules through a computational grid and performs both gas-phase collisions and gas-surface collisions, including chemical reactions. Due to rapidly increasing computer resources the method is now tractable for full-scale engineering problems, and each year its capabilities increase. DSMC holds great potential for molecular-based physics for fluid dynamic modeling involving chemical reactions and gas-surface interactions.

Specifically, funding was used to develop both adaptive mesh refinement (AMR) and 'cut-cell' capability for complex geometry into the DSMC code. The code has been threaded using OpenMP for parallel simulations on shared-memory architectures. Finally, a preliminary MPI version has been implemented for parallel simulations on distributed memory architectures [75, 76, 92, 93, 98].

In order to obtain accurate CFD solutions for hypersonic flows, grids must be aligned with strong gradients in the flow, often requiring an unstructured grid and a user with advanced grid-generation skills. In contrast, accurate DSMC solutions can be obtained on Cartesian grids. This offers a number of advantages for large parallel simulations however, requires “cut-cell” algorithms to cut complex geometry surfaces from a Cartesian flow field grid. Finally, for accuracy and efficiency, DSMC grid cells must be adapted to the local mean free path (proportional to the local density). Essentially the optimal DSMC grid is coupled to the final solution itself and thus naturally requires AMR. The key idea is that both AMR and cut-cell procedures can be fully automated and parallelized in DSMC (Cartesian grids), potentially eliminating the user-time for grid generation. The DSMC code at Minnesota is now able to automatically generate and refine a three-level Cartesian flow field grid around complex 3D geometries and obtain accurate solutions with no user intervention. An example solution for a satellite geometry is shown below.

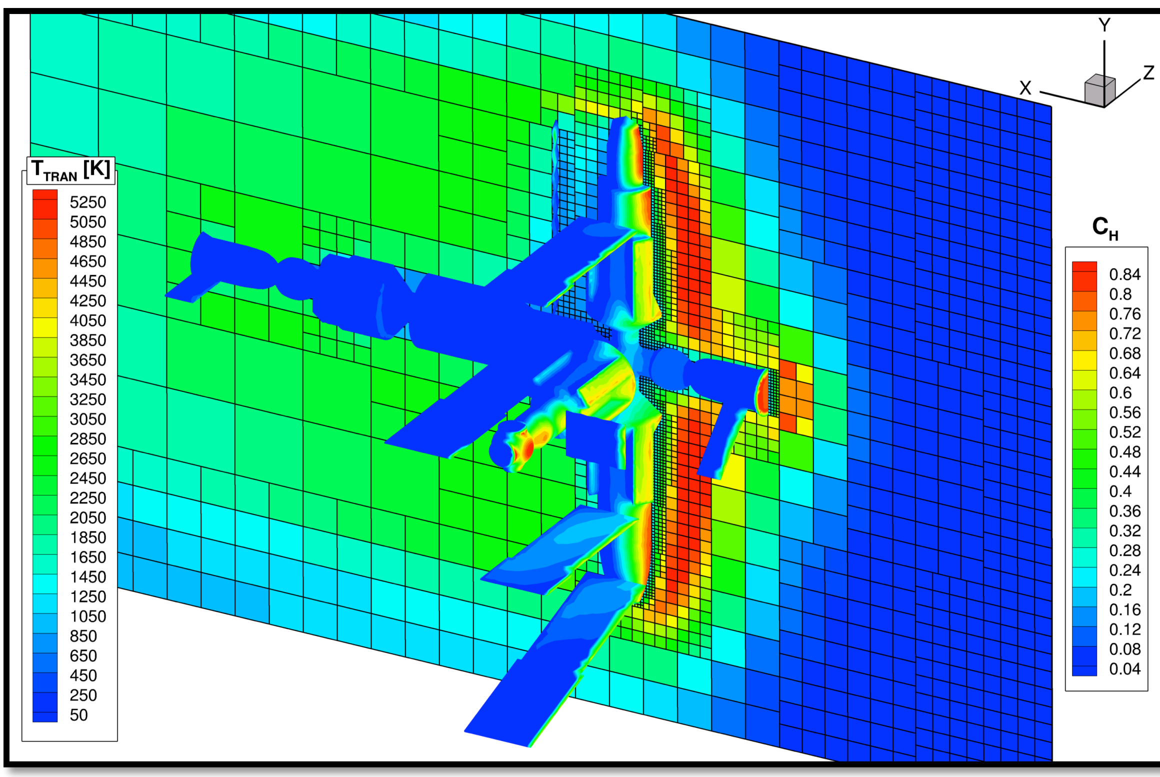


Figure 12. 3D DSMC solution for hypersonic flow over a satellite in low Earth orbit, demonstrating complex geometry capability.

With the mechanics of the DSMC code complete (i.e. surface geometry, flow field grid, particle movement and sorting algorithms), the DSMC method becomes highly modular with respect to physical modeling. Specifically, during a single time step, all chemistry models operate only on the particles within each cell and do not depend on neighboring cells. This enables rapid incorporation of new physical models into the large-scale Minnesota DSMC code. Center funding has partially supported ab-initio computational chemistry research on gas-surface and gas-phase collisions. Specifically, Prof. Schwartzentruber's group has developed a novel accelerated Molecular Dynamics (MD) method specifically for dilute gases. This method enables the efficient simulation of normal shock waves using only atoms and associated inter-atomic potentials (no collision models, transport closures, or rate models). The method has been validated with experimental data for shock waves in argon as well as argon-xenon and argon-helium mixtures. The data produced by such first-principles MD simulations is then used to improve DSMC collision models used in the large-scale Minnesota code. Ongoing work focuses on polyatomic gases including rotation/vibration excitation and dissociation of air in shock layers [64, 65, 67].

Additional Specific Topics Addressed Under Center Support

In the following, additional details concerning specific sub-projects accomplished under Center support are listed in approximate chronological order. Most of this work is supported by detailed publications listed in this report.

1. A new Mach 10 scramjet engine was designed by Center personnel and successfully tested in the CUBRC LENS-I facility in support of the DARPA HyCAUSE program. This engine uses an inward-turning inlet design and is the first such engine ever tested at full scale a fully duplicated flight conditions. Center personnel and computational tools developed at the Center were instrumental in the robust performance obtained from this engine. This inlet/engine concept was flight-tested at the Australian range under support from the HyCAUSE program; unfortunately the flight test was largely unsuccessful because of problems with orienting the flight-test payload during re-entry.

2. The AFOSR STAR program, which was partly funded by Center support, made great progress in transitioning high-fidelity mechanism-based stability analysis tools to the wider community. The STABL tool (Stability and Transition Analysis for hypersonic Boundary Layers) has undergone significant improvements and is now in use at many academic institutions and government labs. STABL was used to predict the transition location on the Lockheed-Martin STAR-1A geometry to support the development of the DARPA FALCON program HTV-1 vehicle. We supported the FALCON HTV-2 aerothermal and transition analysis, and work is underway to analyze transition on the X-51A. STABL is being used to support the Raytheon KEI development program. STABL was also used to study transition to turbulence on the HIFiRE-1 and -5 flight vehicles to design the experiments [12, 24, 34, 46-49, 50, 69].

3. Computational tools developed at the Center were used to support the design of the DARPA FALCON Hypersonic Cruise Vehicle (HCV) inlet and engine flow path.

4. A new low dissipation method for the large-eddy simulation of compressible turbulence has been developed. This approach, which explicitly conserves kinetic energy, captures a

much larger range of length scales than conventional upwind methods. It will enable the LES of compressible turbulent mixing and combustion [63].

5. A novel shock-capturing scheme was developed for unstructured grids; the predictor-corrector approach is applied in the vicinity of detected shock waves. It has the potential to improve solution accuracy and robustness for high-Mach number flows, particularly for direct numerical simulations (DNS) and large-eddy simulations (LES).

6. A new parallel implicit unstructured grid code was developed and validated [5, 11]. This code uses the efficient data-parallel line relaxation approach for unstructured grids, combining the efficiency of structured grid approach with the flexibility of unstructured grids for complex geometry applications. This code, US3D, is becoming widely used; it is now in use at Kirtland AFB in the AFRL Space Vehicles Directorate and at Wright-Patterson AFB in the AFRL Air Vehicles Directorate, as well as at NASA and several academic institutions and industry partners.

7. A nozzle flow analysis tool was developed and released through the AEDC [14]. This code was used to analyze the AEDC Tunnel 9 flow and recent double-cone experiments were simulated at Tunnel 9 flow conditions. Center researchers collaborated closely with AEDC Hypervelocity Tunnel 9 personnel to simulate the Mach 14 nozzle with the goal of understanding its non-ideal performance. As part of this work a novel approach for generating grids in hypervelocity flows was conceived, in which the grid lines are aligned with direction of the characteristics in the supersonic portion of the flow. This approach was shown to resolve small disturbances much more accurately then conventional grids that are not aligned with those weak disturbances. This approach has the potential to greatly improve the accuracy of wind tunnels designs, and more broadly, the simulation of supersonic flows in general [107].

8. New code validation experiments were conducted and the new non-intrusive diagnostics for nitric oxide and water vapor concentration were used to help quantify the flow state in the LENS-I test section [22, 40]. These are the first nitric oxide measurement ever made in the test section of a hypervelocity facility. Work was conducted with the attempt to explain the very puzzling results obtained from the non-intrusive diagnostics measurements. This work has resulted in a series of additional papers; unfortunately, this

problem remains unsolved and will be the subject of part of the proposed computational and experimental program. The present thinking is that the modeling of oxygen recombination in high-enthalpy facility nozzles is significantly inaccurate, which leads to the discrepancies between simulation and experiment. It will take considerably more effort to quantify this effect and to develop predictive models of the recombination process. Furthermore, analysis shows that the electronically excited states may play a role in the recombination process, which will require a complete reformulation of all modeling approaches for high-temperature flows [80, 85, 97].

9. Extensive experimental programs were conducted in the CUBRC facilities, including studies on: high-enthalpy flows over spheres, cylinders, capsules, and double-cones; catalytic heating on capsule configurations; tripping and transition on scramjet engine inlets. Experiments were performed to support the AFRL HiFIRE Flight 1. Extensive simulations were also performed to support these flight experiments. In addition, studies were made to produce comparisons of predicted transition locations on the HIFiRE-1 geometry with measurements in the NASA Langley Mach 6 facility. The key results of these studies are that the e^N approach correlates the HIFiRE-1 configuration data across two very different facilities and very different flow field conditions 34, 46-48, 50]. This is an important result and shows the potential of the mechanism-based stability and transition analysis approach.

10. Under Center support there were modifications and improvements to the LENS-X expansion tunnel for real gas studies at velocities of 10,000 to 27,000 ft/s with significantly reduced issues of test gas reaction. Studies were conducted to make cross-facility comparisons; this work demonstrated that the expansion tunnel is a viable facility for producing extremely high-enthalpy flows with very low freestream contamination and thermo-chemical nonequilibrium. Subsequent studies have confirmed this result with the new CUBRC LENS-XX expansion tunnel facility.

11. A Workshop on Hypersonics was held in Minneapolis September 14-15, 2005.

12. There were extensive interactions with industry, including AeroSystems Engineering, Alliant Tech Systems, Honeywell, Boeing, Lockheed-Martin, Pyrodyne, Aerojet, Northrop-Grumman, Raytheon Missiles and Space, and GoHypersonic Inc.

13. Many papers have been published (approximately 100 conference papers and 35 journal articles); numerous invited and contributed talks were given by Center researchers. Approximately fifteen Ph.D. and 30 M.S. students graduated from the University of Minnesota.

14. The University of Minnesota course in Hypersonic Aerodynamics was extensively updated. The course notes are being put into the format for a textbook on the subject. A new course on Molecular Gas Dynamics was developed by Prof. Schwartzentruber to teach the key aspects of the Direct Simulation Monte Carlo (DSMC) method and concepts in rarefied gas dynamics with application to hypersonic flows at high altitude conditions.

15. Center personnel have served on several advisory committees and panels for NASA, DoD, industry, Sandia National Laboratories, and the Air Force.

16. The Center has been providing support for the HIFiRE Flight 5 vehicle design; this has involved close collaborations with AFRL personnel and resulted in publications documenting the work.

17. Experimental studies have been conducted in the LENS II tunnel to examine the aerothermal characteristics of a scramjet powered hypersonic vehicle designed for Mach 6 flight. Measurements made in these studies are being employed to examine and improve the turbulence modeling used in the DPLR and US3D numerical prediction codes, as well as other standard CFD codes.

18. Extensive experimental studies were conducted in the LENS tunnels in support of the AFOSR HIFiRE and the Air Force FALCON program. Measurements made in these programs were employed to examine the prediction of transition on hypersonic vehicles and to develop improved models of turbulence for predicting regions of shock wave/boundary layer interaction.

19. Experimental studies have continued in the LENS I hypervelocity tunnel to examine the nonequilibrium characteristics of a high-enthalpy flowfield. Analysis of these measurements is continuing with the support of results from numerical prediction

techniques including sophisticated models of flowfield chemistry. Much of this work focused on the double cone configuration.

20. Significant efforts were made in the design and evaluation of the new LENS XX expansion tunnel designed to generate velocities from 10,000 to 27,000 ft/s. In concert with the design of this facility, detailed simulations were made to optimize a contoured nozzle which will meet the requirements of the LENS XX expansion tunnel. The LENS XX facility represents a completely new ground-test capability for high-enthalpy flows. Key aspects are that many re-entry flight conditions can be replicated in the facility, and that the expansion tunnel has very low levels of chemical reaction and internal energy excitation are present in the freestream test gas. This is crucial for high-fidelity testing, radiative emission measurements, and validation-quality data for thermo-chemical model validation and calibration.

21. The Center's computational tools were used to support the design of the DARPA ASET inward-turning inlet. The inlet was optimized and studied under a wide range of flow conditions using Center developed simulation tools; this inlet and flow path was tested at the AEDC Tunnel 9 facility and potentially has application to future hypersonic cruise missile concepts.

22. The University of Minnesota computational fluid dynamics code, US3D, was extended to larger and more complex problems; a recent example simulation used 128 million hexahedral elements and a 5-species finite-rate thermo-chemical model for the Space Shuttle Orbiter flow field. To the best of our knowledge, this is the largest aerothermodynamics simulation ever performed. Other large-scale simulations are being done to support AF programs (HIFiRE-5 and X-51A, for example).

23. A possible explanation for the observed differences in reflected shock tunnel performance and simulations was proposed; this involves a new mechanism in which electronically exited states of oxygen and carbon dioxide are formed during the recombination process in the facility nozzle. New work is progressing to understand and quantify this effect [80, 85, 92, 97].

24. The US3D computational fluid dynamics code was extended to include several new time integration methods required for high order of accuracy simulations. Several new

approaches were investigated and one novel method was developed that shows great promise for wall-modeled large-eddy simulations (WM-LES). This approach makes minor, but critical, modifications to the classic second-order Crank-Nicholson method that provides stability and accuracy for unsteady hypersonic flows. This method has been shown to permit large implicit time steps in the near-wall RANS region, while maintaining accuracy and low dissipation levels in the LES region. This approach is much more cost-effective than competing methods, at least for the certain classes of flows studied under Center support. For example, recent simulations of jets in supersonic cross-flow are enable by this approach.

25. The basic implicit time integration method in US3D was extended from a data-parallel line-relaxation (DPLR) approach to a Generalized Method of Residual (GMRes) method to see if it is possible to improve convergence rates on non-ideal grids and for grids that are not suited to the line-relaxation method. It was found that under some conditions the GMRes method is competitive with the DPLR method, however this very much depends on the type of pre-conditioner used, the optimization of settings for the GMRes method and other details. In general, the DPLR approach works well and in some cases can be made to be significantly faster than GMRes by adjusting the number of sub-iterations used during the relaxation step [44, 103].

26. Related to the GMRes approach, a Newton-like time integration method was also studied with the goal of reducing costs of performing shape optimization on hypersonic inlets, for example. It was found that by converting the DPLR method to a Newton method and using a large number of sub-iteration steps, it is possible to reduce convergence times by a substantial margin for cases in which the flow conditions or geometry do not change much [94, 100]. For example, during a shape optimization, the derivatives of the objective function with respect to geometry variables are required. This requires a baseline CFD simulation and then a series of simulations on slightly perturbed grids. This Newton approach can significantly reduce the cost of the secondary simulations (by approximately a factor of 10), making shape optimization much less computationally demanding. Furthermore, this approach can be used to rapidly investigate aerodynamic performance as a function of flight conditions and/or angle of attack by propagating a solution forward from a baseline simulation.

27. Significant and long-term support was provided through the Center for experiments at the Caltech T5 Free-Piston Shock Tunnel. Center researchers performed numerous computations and interacted closely with Caltech and AFRL personnel to understand the experimental data and to design experiments [61, 82]. The goal of this work was to inject carbon dioxide into a hypervelocity flow to control transition to turbulence. The Center simulated the experiments, performed many STABL analyses of the boundary layers to understand how the CO_2 affected the flow stability and how the injection process could interfere with transition delay by destabilizing the boundary layer. The Center work was extremely important in helping characterize the flow physics and ultimately helped lead to the success of the experiments.

28. Close collaborations between Center researchers and Purdue University personnel resulted in a new understanding of wake transition physics due to discrete roughness elements and protuberances. In particular, detailed, highly-resolved simulations of the Purdue Mach 6 Quiet Tunnel experimental configuration were carried out by Center researchers [88, 102]. Comparisons with experimental data were made; the computations indicated that the source of the dominant frequency of wake unsteadiness originates in the region upstream of the discrete roughness element. Experimental pressure transducers were then placed in that region and were found to measure very similar disturbance properties to that predicted by the simulations. This is probably the first time that a direct numerical simulation was used to make a prediction about a realistic and technically relevant high-speed flow field. This work would not have been possible without the numerical methods and code development performed under Center support.

29. Similar to the above, the US3D code was used to study cross-flow transition on a cone at conditions relevant to the Purdue Mach 6 Quiet Tunnel flow [105]. Simulations produced cross-flow disturbances that are similar to those observed in wind tunnel measurements. This work is still preliminary, but shows the potential for direct simulations of this type of transition mechanism in hypersonic flows.

30. A very large body of work was conducted related to wall-modeled large-eddy simulations (WM-LES), with emphasis on fuel-air mixing simulations at technologically relevant conditions [21, 25, 28, 30, 38, 55, 57, 71, 74, 89, 96, 99, 101, 108]. This work

has shown that with the use of appropriate low-dissipation high-order of accuracy numerical methods, large high-quality carefully designed grids, and certain variants of turbulence models and inflow conditions, it is possible to reproduce experimental data for fuel-air mixing. This is an extremely important conclusion because it paves the way for detailed simulations of actual combustor configurations, and ultimately for the optimization of hypersonic air-breathing propulsion system flow paths. This is a major accomplishment of the Center and has the potential to revolutionize the efficiency and robustness of future propulsion systems. We are now working to transition this capability to the AFRL and to potential industry users.

31. Related to the above accomplishment, Center funds were used to develop an experimental configuration for obtaining high-quality open-literature data for code validation of fuel-air mixing and combustion at relevant conditions and with multiple interacting injection ports. This "combustion duct" was designed to have some similarity to the AFRL HIFiRE-2 flight experiment configuration, but is completely generic and is not in any way optimized to produce a high-quality flight system relevant flow. It uses simple angled round injection ports and can be configured in many different ways to allow specific data to be obtained. Up to 9 individual fuel injection ports may be operated. The experimental rig has optical access that will enable laser-based diagnostics to be used to characterize the flow field. Initial experiments were run at CUBRC and new experiments are planned with additional diagnostics methods in place to extend the value of the data. At the University of Minnesota, the CUBRC combustion duct has been simulated using the WM-LES approach with various injector configurations in place, and at several flow conditions. Initial comparisons with the limited experimental data are very encouraging [101]. If it is possible to obtain agreement between simulation and experiment for this configuration, it will provide confidence that the numerical methods and turbulence modeling approaches can be used for system-relevant air-breathing propulsion systems.

32. As the WM-LES approaches and associated numerical methods have gained maturity, Center researchers have begun to perform direct numerical simulations (DNS) of hypersonic turbulent flows. This approach, which resolves all physically-relevant length and time scales, promises to provide statistically exact data of important turbulent flows.

For example, a puzzling result has been observed on the HIFiRE-1 blunt cone configuration. Here, the measured turbulent heat flux is best predicted with a very simple (Baldwin-Lowmax) turbulence model, while more physically-relevant models over-predict the measured heat flux by substantial margins. This is of course a major concern and has serious implications for system design uncertainty and thermal protection system sizing. Through Center support, it is now possible to perform DNS of these flows at actual wind tunnel conditions; though these simulations are time-consuming (requiring about 2 months on 1000 processor cores with a 300 million element grid) , they have the potential to improve the turbulence models and explain why the heat flux is so poorly predicted. This capability should enable new simulations to help explain many outstanding problems in hypersonic flow physics.

33. Related to the WM-LES and DNS capability, is the area of chemistry-turbulence interactions. As described above, it is now possible to predict fuel-air mixing in practical supersonic air-breathing propulsion configurations. However, a major issue remains: how to model the interaction of turbulent motion with chemical reactions and the combustion process in general. A huge body of work exists for the modeling of this interaction at low-speed combustion conditions, but there is no accepted approach for high-speed (supersonic) flow conditions. Because of the high speeds, the relative time scales of fluid motion and chemical reaction are considerably different and thus the well-established models cannot be applied without modification. Under Center support, work in this area was initiated, but was not completed. The US3D code was modified to allow Lagrangian particle tracking so that a Filtered Mass Density Function (FMDF) approach can be used to represent subgrid scale chemistry-turbulence interactions in a large-eddy simulation approach; the FMDF approach has been very successful at low speeds and should be readily adaptable to the high-speed flow environment. With further development this approach shows promise for providing a rigorous chemistry-turbulence interaction closure.

34. A novel accelerated molecular dynamics (MD) approach was developed that allows low-density flows to be simulated at a near first-principles level. The accelerated MD collapses the simulation time that occurs between collisions so that the simulations do not compute the particle interactions when they are not interacting and are on ballistic

trajectories. This is an important advance and will enable new much more detailed simulations of critical physical processes in high-temperature flows. An important application is to shock waves so as to better understand the physics that occur within the highly nonequilibrium region associated with a shock wave [64, 65, 67].

ACKNOWLEDGEMENT AND DISCLAIMER

This work was sponsored (in part) by the Air Force Office of Scientific Research, USAF, under grant/contract numbers FA9550-04-1-0341 and FA9550-10-0352. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the Air Force Office of Scientific Research or the U.S. Government.

PUBLICATIONS

[1] Nompelis, I., G.V. Candler and M.S. Holden, “Effect of Vibrational Nonequilibrium on Hypersonic Double-Cone Experiments,” *AIAA Journal*, Vol. 41, No. 11, pp. 2162-2169, Nov. 2003.

[2] Sun, Q., I.D. Boyd, and G.V. Candler, “A Hybrid Continuum/Particle Approach for Modeling Subsonic, Rarefied Gas Flows,” *Journal of Computational Physics*, Vol. 194, No. 1, pp. 256-277, Feb. 2004.

[3] Nompelis, I., G.V. Candler, and M.S. Holden, “Numerical Simulation of High-Enthalpy Double-Cone Experiments in the LENS X Expansion Tube Facility,” AIAA Paper 2004-1000, Jan. 2004.

[4] Sinha, K., K. Mahesh, and G.V. Candler, “Effect of Shock Unsteadiness on Shock Wave / Turbulent Boundary Layer Interaction,” AIAA Paper 2004-1129, Jan. 2004.

[5] Nompelis, I., T. Drayna, and G.V. Candler, “Development of a Hybrid Unstructured Implicit Solver for the Simulation of Reacting Flows Over Complex Geometries,” AIAA 2004-2227, June 2004.

[6] Stecher, J., and G. Candler, "Computational Analysis of Laminar Boundary Layer Separation on a Slender Cone at Angle of Attack," AIAA-2005-509, Jan. 2005.

[7] Nompelis, I., G.V. Candler, M. MacLean, T. Wadhams and M. Holden, "Numerical Investigation of High Enthalpy Chemistry on Hypersonic Double-Cone Experiments," AIAA-2005-584, Jan. 2005.

[8] Coblish, J. and M. Smith, T. Hand, I. Nompelis, and G.V. Candler, “Double-Cone Experiment and Numerical Analysis at AEDC Hypervelocity Wind Tunnel No. 9,” AIAA-2005-0902, Jan. 2005.

[9] MacLean, M., G. Candler, and M. Holden, "Numerical Evaluation of Flow Conditions in the LENS Reflected Shock-Tunnel Facilities," AIAA-2005-903, Jan. 2005.

[10] Holden, M., T. Wadhams, and M. MacLean, "Experimental Studies to Examine Viscous/Inviscid Interactions and Flow Chemistry Effects of Hypersonic Vehicle Performance," AIAA-2005-4694, June 2005.

[11] Nompelis, I., T. Drayna and G.V. Candler, "A Parallel Unstructured Implicit Solver for Hypersonic Reacting Flow Simulation," AIAA-2005-4867, June 2005.

[12] Johnson, H.B., and G. Candler, "Hypersonic Boundary Layer Stability Analysis Using PSE-Chem," AIAA-2005-5023, June 2005.

[13] Wan, T., R. Suzuki, G.V. Candler, S. Macheret and M. Shneider, "Three Dimensional Simulation of Electric Field and MHD Power Generation During Re-Entry," AIAA-2005-5045, June 2005.

[14] Candler, G.V., "Hypersonic Nozzle Analysis Using an Excluded Volume Equation of State," AIAA-2005-5202, June 2005.

[15] Sinha, K., K. Mahesh, and G.V. Candler, "Modeling the Effect of Shock Unsteadiness in Shock/ Turbulent Boundary-Layer Interactions," *AIAA Journal*, Vol. 43, No. 3, pp. 586-594, 2005.

[16] Druguet, M.-C., G.V. Candler, and I. Nompelis, "Effects of Numerics on Navier-Stokes Computations of Hypersonic Double-Cone Flows," *AIAA Journal*, Vol. 43, No. 3, pp. 616-623, 2005.

[17] Hou Y., and K. Mahesh, "A Robust Colocated Implicit Algorithm for Direct Numerical Simulation of Compressible Turbulent Flows," *Journal of Computational Physics*, Vol. 205, No. 1, pp. 205-221, 2005.

[18] MacLean, M., and M. Holden, "Catalytic Effects on Heat Transfer Measurements for Aerothermal Studies with CO2," AIAA-2006-182, Jan. 2006.

[19] Drayna, T., I. Nompelis and G.V. Candler, "Hypersonic Inward Turning Inlets: Design and Optimization," AIAA-2006-297, Jan. 2006.

[20] Holden, M., "Historical Review of Experimental Studies and Prediction Methods to Describe Laminar and Turbulent Shock Wave/Boundary Layer Interactions in Hypersonic Flows," AIAA-2006-494, Jan. 2006.

[21] Peterson, D., P. Subbareddy, and G.V. Candler, "DES Investigation of Transverse Injection into Supersonic Crossflow using a Hybrid Unstructured Solver," AIAA-2006-903, Jan. 2006.

[22] Parker, R., T. Wakeman, M. Holden and M. MacLean, "Measuring Nitric Oxide Freestream Concentration Using Quantum Cascade Lasers at CUBRC," AIAA-2006-926, Jan. 2006.

[23] Drayna, T., I. Nompelis, and G.V. Candler, "Numerical Simulation of the AEDC Waverider at Mach 8," AIAA-2006-2816, June 2006.

[24] Johnson, H.B., and G. Candler, "Analysis of Laminar-Turbulent Transition in Hypersonic Flight Using PSE-Chem," AIAA-2006-3057, June 2006.

[25] Peterson, D., P. Subbareddy and G.V. Candler, "Simulation of Injection Into a Supersonic Crossflow using DES with Synthetic Inflow," AIAA-2006-3326, June 2006.

[26] Druguet, M.-C., G.V. Candler and I. Nompelis, "Comparison of Physical Models in Computations of High-Enthalpy Double-Cone Flows," AIAA-2006-3419, June 2006.

[27] Subbareddy, P., D. Peterson, G.V. Candler and I. Marusic, "A Synthetic Inflow Generation Method Using the Attached Eddy Hypothesis," AIAA-2006-3672, June 2006.

[28] Peterson, D., P. Subbareddy, and G.V. Candler, "Detached Eddy Simulations of Flush Wall Injection into a Supersonic Freestream," AIAA-2006-4576, July 2006.

[29] Holden, M., T. Wadhams, and M. MacLean, "Experimental Studies to Examine Viscous/Inviscid Interactions and Flow Chemistry Effects of Hypersonic Vehicle Performance," AIAA-2005-4694, June 2006.

[30] Peterson, D., P. Subbareddy and G.V. Candler, "Assessment of Synthetic Inflow Generation for Simulating Injection Into a Supersonic Crossflow," AIAA-2006-8128, Nov. 2006.

[31] MacLean, M., M. Holden, T. Wadhams, R. Parker, "A Computational Analysis of Thermochemical Studies in the LENS Facilities," AIAA-2007-121, Jan. 2007.

[32] Nompelis, I., and G.V. Candler, "Investigation of Hypersonic Double-Cone Flow Experiments at High Enthalpy in the LENS Facility," AIAA-2007-203, Jan. 2007.

[33] Holden, M., T. Wadhams, M. MacLean, E. Mundy, and R. Parker, "Experimental Studies in LENS I and X to Evaluate Real Gas Effects on Hypevelocity Vehicle Performance," AIAA-2007-204, Jan. 2007.

[34] Johnson, H.B., C. Alba, G.V. Candler, M. MacLean, T. Wadhams and M. Holden, "Boundary Layer Stability Analysis to Support the HIFiRE Transition Experiment," AIAA-2007-311, Jan. 2007.

[35] Wan, T., G.V. Candler, and R. Suzuki, "Computational Simulation of Magnetohydrodynamics Acceleration Experiments Using Newton-Krylov-Schwarz Method," AIAA-2007-393, Jan. 2007.

[36] Hash, D., J. Olejniczak, M. Wright, D. Prabhu, M. Pulsonetti, B. Hollis, P. Gnoffo, M. Barnhardt, I. Nompelis, and G.V. Candler, "FIRE II Calculations for Hypersonic Nonequilibrium Aerothermodynamics Code Verification: DPLR, LAURA, and US3D," AIAA-2007-605, Jan. 2007.

[37] Park, N. and K. Mahesh, "Numerical and Modeling Issues in LES of Compressible Turbulence on Unstructured Grids," AIAA-2007-722, Jan. 2007.

[38] Sinha, K., and G.V. Candler, "Grid Sensitivity of Detached Eddy Simulation of a Mach 16 Re-Entry Configuration," AIAA-2007-1115, Jan. 2007.

[39] Holden, M., T. Wadhams and M. MacLean, "Experimental Studies in Hypersonic Flows for Facility and Code Validation," AIAA-2007-1304, Jan. 2007.

[40] Parker, R. and T. Wakeman, M. MacLean and M. Holden, "Measuring Nitric Oxide Freestream Velocity Using Quantum Cascade Lasers at CUBRC," AIAA-2007-1329, Jan. 2007.

[41] Doom, J., and K. Mahesh, "A Numerical Method for DNS/LES of Turbulent Reacting Flows," AIAA-2007-1415, Jan. 2007.

[42] Candler, G.V., "Unstructured Grid Approaches for Accurate Aeroheating Simulations (Invited)," AIAA-2007-3959, June 2007.

[43] Gidzak, V., I. Nompelis and G.V. Candler, "Development of Stencil-Based Mesh Partitioning for Parallel Unstructured CFD Solvers," AIAA-2007-4087, June 2007.

[44] Nompelis, I., T. Wan and G.V. Candler, "Performance Comparisons of Parallel Implicit Solvers for Hypersonic Flow Computations on Unstructured Meshes," AIAA-2007-4334, June 2007

[45] Wan, T., and G.V. Candler, "High Performance Parallel Implicit Computations of Three-dimensional Supersonic Magnetohydrodynamics Using PETSc Library," AIAA-2007-4367, June 2007.

[46] Wadhams, T., M. MacLean, M. Holden and E. Mundy, "Full Scale Ground Testing of the FRESH FX-1 at Flight Duplicated Conditions," AIAA-2007-4488, June 2007.

[47] MacLean, M., E. Mundy, T. Wadhams, M. Holden, H. Johnson and G.V. Candler, "Comparisons of Transition Prediction Using PSE-Chem to Measurements for a Shock Tunnel Environment," AIAA-2007-4490, June 2007.

[48] Alba, C., H. Johnson, M. Bartkowicz, and G.V. Candler, "Boundary Layer Stability Calculations of the HIFiRE Flight 1 Vehicle in the LaRC 20-Inch Mach 6 Air Tunnel," AIAA-2008-505, Jan. 2008.

[49] Ozawa, T., I. Nompelis, D. Levin, M. Barnhardt and G.V. Candler, "DSMC-CFD Comparison of a High Altitude, Extreme-Mach Number Reentry Flow," AIAA-2008-1216, Jan. 2008.

[50] Johnson, H.B., C. Alba, G.V. Candler, M. MacLean, T. Wadhams, and M.S. Holden, "Boundary-Layer Stability Analysis of the Hypersonic International Flight Research Transition Experiments," Journal of Spacecraft and Rockets, Vol. 45, No. 2, pp. 228-236, March-April 2008.

[51] Candler, G.V., and T. Drayna, "Design and Optimization of the ASET Inward-Turning Scramjet Inlet," JANNAF 30th Airbreathing Propulsion Subcommittee Meeting, Boston, May 2008.

[52] Gosse, R., and G.V. Candler, "Evaluation of Carbon-Carbon Ablation Models Using a Fully Coupled CFD Solver," AIAA-2008-3908, June 2008.

[53] Alba, C., H.B. Johnson and G.V. Candler, "Oblique Wave Disturbance Analysis of Supersonic Flow Past Axisymmetric and 2D Bodies at Angles of Attack," AIAA-2008-4396, June 2008.

[54] Johnson, H.B., M. Bartkowicz, T.W. Drayna, G.V. Candler and C. Alba, "Design Optimization of Hypersonic Vehicles for Boundary Layer Stability," AIAA-2008-6221, Aug. 2008.

[55] Peterson, D., and G.V. Candler, "Hybrid RANS/LES of a Supersonic Combustor," AIAA-2008-6923, Aug. 2008.

[56] Candler, G.V., C. Alba, and H.B. Johnson, "Computational Prediction of HTV-2 Aerodynamics and Aerothermal Environment," AIAA Missile Sciences Conference, Nov. 2008.

[57] Candler, G.V., D. Peterson and T. Drayna, "Detached Eddy Simulation of a Generic Scramjet Inlet and Combustor," AIAA-2009-0130, Jan. 2009.

[58] Candler, G.V., D. Mavriplis, "Current Status and Future Prospects for the Numerical Simulation of Hypersonic Flows," AIAA-2009-0153, Jan. 2009.

[59] MacLean, M., E. Mundy, T. Wadhams, M. Holden, M. Barnhardt, and G.V. Candler, "Experimental and Numerical Study of Laminar and Turbulent Base Flow on a Spherical Capsule," AIAA-2009-783, June 2009.

[60] Johnson, H.B., J. Gronvall and G.V. Candler, "Reacting Hypersonic Boundary Layer Stability with Blowing and Suction," AIAA-2009-0938, Jan. 2009.

[61] Leyva, I. R. Wagnild, H.G. Hornung, G.V. Candler, "Transition Delay in Hypervelocity Boundary Layers by Means of CO2/Acoustic Instability Interactions," AIAA-2009-1287, Jan. 2009.

[62] Doraiswamy, S. D. Kelley, G.V. Candler, "Vibrational Modeling of CO_2 in High Enthalpy Nozzle Flows," AIAA-2009-1570, Jan. 2009.

[63] Subbareddy, P., and G.V. Candler, "A Fully-Discrete, Kinetic Energy Consistent Finite Volume Scheme for Compressible Flows," *Journal of Computational Physics*, Vol. 228, pp. 1347-1364, Mar. 2009.

[64] Valentini, P. and Schwartzentruber, T.E., "Combined Event-Driven/Time-Driven Molecular Dynamics Algorithm for the Simulation of Shock Waves in Rarefied Gases," *Journal of Computational Physics*, 228, 8766-8778, 2009.

[65] Valentini, P. and Schwartzentruber, T.E., "Large-scale Molecular Dynamics Simulations of Normal Shock Waves in Dilute Argon", *Physics of Fluids*, 21, 066101, pp. 1-9, 2009.

[66] Wan, T., G.V. Candler, S.O. Macheret, and M. Shneider, "Three Dimensional Simulation of Electric Field and MHD Power Generation During Reentry," *AIAA Journal*, Vol. 47, No. 6, pp. 1327-1336, June 2009.

[67] Schwartzentruber, T.E., and Valentini, P., "Molecular Dynamics Simulations of Normal Shocks in Dilute Gases," AIAA Paper 2009-3602, June 2009.

[68] Candler, G.V., "Comparison of CFD and Theoretical Post-Shock Gradients in Hypersonic Flow," AIAA-2009-3719, June 2009.

[69] Choudhari, M., C.-L. Chang, T. Jentink, F. Li, K. Berger, G.V. Candler, and R. Kimmel, "Transition Analysis for the HIFiRE-5 Vehicle," AIAA-2009-4056, June 2009.

[70] Doraiswamy, S., J.D. Kelley, and G.V. Candler, "Vibrational Modeling of CO_2 in High-Enthalpy Nozzle Flows," *Journal of Thermophysics and Heat Transfer*, Vol. 24, No. 1, pp. 9-17, Jan. 2010.

[71] Peterson, D., and G.V. Candler, "Hybrid RANS/LES of Normal Injection into a Supersonic Crossflow," *Journal of Propulsion and Power*, Vol. 26, No. 3, pp. 533-544, Mar. 2010.

[72] Sharma, M., A. Swantek, W. Flaherty, J. Austin, S. Doraiswamy, G.V. Candler, "Experimental and Numerical Investigation of Hypervelocity Carbon Dioxide Flow over Blunt Bodies," *Journal of Thermophysics and Heat Transfer*, Vol. 24, No. 4 pp. 673-683, Oct.-Dec. 2010.

[73] Ozawa, T., D. Levin, I. Nompelis, M. Barnhardt, G.V. Candler, "Particle and Continuum Method Comparison of a High-Altitude, Extreme-Mach-Number Reentry Flow," *Journal of Thermophysics and Heat Transfer*, Vol. 24, No. 2, 2010.

[74] Peterson, D., and G.V. Candler, "Supersonic Combustor Simulations Using a Hybrid RANS/LES Approach," AIAA-2010-0411, Jan. 2010.

[75] Gao, D., Zhang, C., and Schwartzentruber, T.E., “Three-Level Cartesian Geometry-Based Implementation of the DSMC Method,” AIAA Paper 2010-0450, Jan. 2010.

[76] Gao, D. and Schwartzentruber, T.E., “Parallel Implementation of the Direct Simulation Monte Carlo Method for Shared Memory Architectures,” AIAA Paper 2010-0451, Jan. 2010.

[77] Candler, G.V., "Hypersonic Navier Stokes Comparisons to Orbiter Flight Data," AIAA-2010-0455, Jan. 2010.

[78] Johnson, H.B., and G.V. Candler, "Orbiter Boundary Layer Transition Stability Modeling at Flight Entry Conditions," AIAA-2010-0457, Jan. 2010.

[79] Gronvall, J., H. Johnson and G.V. Candler, "Boundary Layer Stability Analysis of the Free-Piston Shock Tunnel HIEST Transition Experiments," AIAA-2010-0896, Jan. 2010.

[80] Candler, G.V., S. Doraiswamy, I. Nompelis and J.D. Kelley, "The Role of Electronically-Excited States in Recombining Flows," AIAA-2010-0912, Jan. 2010.

[81] Bartkowicz, M., P. Subbareddy and G.V. Candler, "Simulation of Boundary Layer Transition on Elliptic Cones in Hypersonic Flow," AIAA-2010-1064, Jan. 2010.

[82] Wagnild, R., G.V. Candler, J. Jewell and H. Hornung, "Carbon Dioxide Injection for Hypervelocity Boundary Layer Stability," AIAA-2010-1244, Jan. 2010.

[83] Holden, M.; Wadhams, T.; and MacLean, M. “A Review of Experimental Studies with the Double Cone and Hollow Cylinder/Flare Configurations in the LENS Hypervelocity Tunnels and Comparisons with Navier-Stokes and DSMC Computations,” AIAA 2010-1281, Jan. 2010.

[84] Nompelis, I., and G.V. Candler, "Numerical Investigation of Double-Cone Flow Experiments with High-Enthalpy Effects," AIAA-2010-1283, Jan. 2010.

[85] Doraiswamy, S., J.D. Kelley and G.V. Candler, "Analysis of Chemistry-Vibration Coupling in Diatomics for High Enthalpy Nozzle Flows," AIAA-2010-1570, Jan. 2010.

[86] Candler, G.V., "Comparison of CFD and Theoretical Post-Shock Gradients in Hypersonic Flow," *Progress in Aerospace Sciences*, Vol. 46, No. 2-3, pp. 81-86, Feb.-Apr. 2010.

[87] Valentini, P., Schwartzentruber, T.E., and Cozmuta, I., “Molecular dynamics simulation of O_2 sticking on Pt(111) using the ab initio based ReaxFF reactive force field”, *Journal of Chemical Physics*, 133 (2010) 084703.

[88] Bartkowicz, M., P. Subbareddy, and G.V. Candler, "Numerical Simulations of Roughness Induced Instability in the Purdue Mach 6 Wind Tunnel," AIAA-2010-4723, June 2010.

[89] Tylczak, E., D. Peterson, and G.V. Candler, "Hybrid RANS/LES Simulation of Transverse Jet in Supersonic Crossflow with Laser Energy Deposition," AIAA-2010-4856, June 2010.

[90] Johnson, H., G.V. Candler, C. Alba, "Three-Dimensional Hypersonic Boundary Layer Stability Analysis with STABL-3D," AIAA-2010-5005, June 2010.

[91] Valentini, P., Schwartzentruber, T.E., and Cozmuta, I., "Molecular Dynamics modeling of O2/Pt(111) gas-surface interaction using the ReaxFF potential", proceedings of the 27th International Symposium on Rarefied Gas Dynamics, July 2010, Monterey, CA.

[92] Gao, D., Zhang, C., and Schwartzentruber, T.E., "Particle Simulations of Planetary Probe Flows Employing Automated Mesh Refinement", *Journal of Spacecraft and Rockets*, Vol. 48, No. 3, 2011.

[93] Gao, D. and Schwartzentruber, T.E., "Optimizations and OpenMP Implementation for the Direct Simulation Monte Carlo Method", *Computers and Fluids*, 42, pp. 73-81, 2011.

[94] Drayna, T., G.V. Candler, and H. Johnson, "A Nonlinear Sensitivity Solver for Aerodynamic Shape Optimization and Rapid Design Space Exploration," AIAA-2011-26, Jan. 2011.

[95] Sharma, M., A. Swantek, W. Flaherty, J. Austin, S. Doraiswamy, and G.V. Candler, "Evaluation of Hypervelocity Carbon Dioxide Blunt Body Experiments in an Expansion Tube Facility," AIAA-2011-136, Jan. 2011.

[96] Tylczak, E., G.V. Candler, D. Peterson, "Simulation of Plasma-Spark-Enhanced Mixing in Jet in Supersonic Crossflow," AIAA-2011-398, Jan. 2011.

[97] Doraiswamy, S., D. Kelley, and G.V. Candler, "Energy Bin based Coupling Model for High Enthalpy Flows Using Prior Recombination Distribution," AIAA-2011-450, Jan. 2011.

[98] Gao, D. and Schwartzentruber, T.E., "A Parallel DSMC Implementation Including Adaptive Mesh Refinement and Cut-Cell Algorithms", AIAA Paper 2011-0633, Jan. 2011.

[99] Peterson, D., E. Tylczak, G.V. Candler, "Hybrid Reynolds-Averaged and Large-Eddy Simulation of Scramjet Fuel Injection," AIAA-2011-2344, April 2011.

[100] Stern, E., and G.V. Candler, "Implementation of a Newton Method for the Rapid Propagation of Thermochemical Model Uncertainty in Hypersonic Flows," AIAA-2011-3146, June 2011.

[101] Tylczak, E.B., D.M. Peterson, and G.V. Candler, "Hybrid RANS/LES Simulation of Injection and Mixing in the CUBRC Combustion Duct," AIAA-2011-3216, June 2011.

[102] Wheaton, B., S.P, Schneider, M. Bartkowicz, P. Subbareddy, G.V. Candler, "Roughness-Induced Instabilities at Mach 6: A Combined Numerical and Experimental Study," AIAA-2011-3248, June 2011.

[103] Nompelis, I., J. Bender, and G.V. Candler, "Implementation and Comparisons of Parallel Implicit Solvers for Hypersonic Flow Computations on Unstructured Meshes," AIAA-2011-3547, June 2011.

[104] Wagnild, R., G.V. Candler, "Direct Numerical Simulation of Transient Growth on a Flat Plate at Mach 3," AIAA-2011-3560, June 2011.

[105] Gronvall, J., H.B. Johnson, and G.V. Candler, "Hypersonic Three-Dimensional Boundary Layer Transition on a Cone at 6.0^{o} Angle of Attack," AIAA-2011-3561, June 2011.

[106] Subbareddy, P., and G.V. Candler, "DNS of Transition to Turbulence in a Hypersonic Boundary Layer," AIAA-2011-3564, June 2011.

[107] Boe, K., and G.V. Candler, "A Novel Simulation Approach for the AEDC Hypervelocity Tunnel 9 Mach 14 Nozzle, AIAA-2011-3888, June 2011.

[108] Peterson, D., and G.V. Candler, "Numerical Simulations of Mixing for Normal and Low-Angled Injection into a Mach 2 Crossflow," *AIAA Journal*, Vol. 49, No. 12, pp. 2792-2804, Dec. 2011.

AIR FORCE RELATED TRANSITIONS

The nozzle flow simulation CFD code has been transitioned to the Arnold Engineering and Development Center (AEDC) for analysis of the flow in the Aero-Propulsion Test Unit (APTU) and Tunnel 9.

Extensive simulations of the AEDC Tunnel 9 nozzle flow were conducted and double-cone experiments were designed for the facility. Computations were performed to support the analysis of the double cone experiments.

The STABL (Stability and Transtion Analysis for hypersonic Boundary Layers) code has been transitioned to many sites including AFRL Air Vehicles, Wright-Patterson AFB. The code is in active use at these institutions for hypersonic transition analysis and comparison to flight and ground test data, including several contractors that are using STABL for AF and other DoD work.

The US3D code has been transitioned to AFRL Space Vehicles, Kirtland AFB and AFRL Air Vehicles, Wright-Patterson AFB.

There were extensive interactions and collaborations between Center researchers and Caltech and AFRL Propulsion Directorate, Edwards AFB.

Graduate students and researchers spent time during the summer at Wright-Patterson AFB working with AFRL personnel.